




# Bharathiar University

State University | "A<sup>++</sup>" Grade by NAAC | 46<sup>th</sup> Rank in MoE-NIRF  
Maruthamalai Road, Coimbatore, Tamil Nadu - 641 046.

<b>Dr K. SENTHILKUMAR</b> Professor Department of Physics Bharathiar University Coimbatore, 641046 Tamil Nadu, India <b>E-mail:</b> ksenthil@buc.edu.in <b>Phone:</b> 9486411335 <b>Office Number:</b> 04222428448	
<b>Research Area</b> <ul style="list-style-type: none"><li>• Molecular Quantum Mechanics</li><li>• Computational Material Science</li><li>• Structure Property Relationship</li></ul>	<b>Courses Teaching</b> <ul style="list-style-type: none"><li>• Thermodynamics and statistical mechanics</li><li>• Quantum mechanics</li><li>• Numerical Methods</li><li>• Computer programming with ForTran and Python</li><li>• Molecular Quantum Mechanics</li></ul>
<b>Research Experience:</b> 23	<b>Teaching Experience:</b> 19
<b>Research Credentials</b> (as on February 2026 – Source: Google scholar) H-index: 31                      Citations: 4375                      i10-index: 87	
<b>Patents :</b> Granted: 1	
<b>Publications</b> International Journals: 142                      National Journals: 1                      Books/Chapters: 3 Conferences: 11	
<b>Career</b> <b>At Bharathiar University</b> <ol style="list-style-type: none"><li><b>1. Designation : Professor</b> Period : January 2021 - Till Date</li><li><b>2. Designation : Associate Professor</b> Period : January 2018 - January 2021</li><li><b>3. Designation : Assistant Professor</b> Period : January 2008 - January 2018</li></ol> <b>Other Institutes</b> <ol style="list-style-type: none"><li><b>1. Designation : Lecturer</b> Institution Name : N. G. M. College, Pollachi Period : September 2006 - January 2008</li><li><b>2. Designation : Post Doctoral Fellow</b> Institution Name : Bristol University, United Kingdom Period : August 2005 - August 2006</li><li><b>3. Designation : Post Doctoral Fellow</b> Institution Name : Delft University of Technology, The Netherlands Period : August 2002 - June 2005</li></ol>	
<b>Education</b> <b>Ph. D.</b> Subject : Physics Institution : Bharathiar University, Coimbatore - 641 046 Affiliated University : Bharathiar University, Coimbatore - 641 046 Year of Award : June 2002	



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Maruthamalai Road, Coimbatore, Tamil Nadu - 641 046.

Dr K. SENTHILKUMAR , Professor , Department of Physics

## M. Phil.

Subject : Physics

Institution : Bharathiar University, Coimbatore - 641 046

Affiliated University : Bharathiar University, Coimbatore - 641 046

Year of Award : May 1999

## M. Sc.

Subject : Physics

Institution : Nallamuthu Gounder Mahalingam College, Pollachi - 642 001

Affiliated University : Bharathiar University, Coimbatore - 641 046

Year of Award : May 1997

## B. Sc.

Subject : Physics

Institution : Nallamuthu Gounder Mahalingam College, Pollachi - 642 001

Affiliated University : Bharathiar University, Coimbatore - 641 046

Year of Award : May 1995

## Projects

### National Level

Ongoing - completed - 5

## Research Guidance

### Completed

Ph.D. - 13 M.Phil. - 19 PG - 41

### On Going

Ph.D. - 2

## Institutional Responsibilities

### Coordinator - Centre for internet and website services

Period :Sep 2011 - Jul 2025

Nature of Responsibility :Taking care of University LAN, Internet, and website

### Nodal Officer

Period :Jun 2022 to Till date

Nature of Responsibility :UGC - Students Grievance

## Visits

1. Visiting Scientist at Beijing computational science research center, Beijing, China ( 2017-06-10 - 2017-06-17 )
2. International Congress on Quantum Chemistry 2009 at University of Helsinki, Finland ( 2009-06-22 - 2009-06-27 )
3. Post Doctoral Research Associate at Bristol University, United Kingdom ( 2005-08-01 - 2006-08-01 )
4. Group Symposium on Molecular simulation at Molecular Biophysics, IWR, University of Heidelberg, Heidelberg, Germany ( 2008-03-21 - 2008-03-21 )
5. Sixth international symposium on functional Pi- electron systems at Cornell University, Ithaca, New York, USA ( 2004-06-13 - 2004-06-18 )
6. European Summer School in Quantum Chemistry at Tjornarp Conference Centre, Tjornarp Org. by Department of Theoretical Chemistry, University of Lund, Sweden ( 2003-08-17 - 2003-08-30 )
7. Post Doctoral Researcher at Delft University of Technology, The Netherlands ( 2002-08-01 - 2005-06-01 )
8. Spring college in Numerical methods in electronic structure theory at the Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy ( 2001-05-07 - 2001-05-25 )

## Collaborations

1. Dr. R. Karvembu, Professor, Department of Chemistry, National Institute of Technology, Trichy-620 015
2. Dr. D. Nataraj, Professor, Department of Physics, Bharathiar University, Coimbatore- 641046
3. Dr. Daniel Thangadurai, Professor, Department of Chemistry, KPR Institute of Engineering and Technology, Coimbatore -641 407



4. Dr. L. Sandhiya, Scientist, CSIR-National Institute of Science Communication and Policy Research, New Delhi 110012.

## Programs organized

1. DST-SERB supported online workshop on electronic structure calculations for molecules and materials ( 2023-04-17 - 2023-04-24 )
2. DST-PURSE supported satellite symposium on physical sciences ( 2022-09-13 - 2022-09-15 )
3. Refresher course in physics ( 2014-12-03 - 2014-12-23 )
4. Workshop on theoretical physics ( 2013-12-09 - 2013-12-12 )
5. Workshop on theoretical physics ( 2012-12-17 - 2012-12-20 )
6. Workshop on theoretical physics ( 2011-12-19 - 2012-12-22 )

## Publications

### International Journals - 142

#### 142. Aza-triphenylene and benzene based COF as an anode for Na and Mg ion batteries

Applied Surface Science 719, 165052 (February 2026)

V. M. Vasanthakannan, K. Senthilkumar

#### 141. Exploring the potential of ruthenium(II) cyclometallated complexes encompassing multifaced CNS pincer

##### Schiff base ligands as catalysts in one-pot synthesis of quinolones

Journal of Molecular Structure 1353, 144756 (February 2026)

R. Krishnapriya, S. Gayathri, Priya Raj Murugesan, Jagathesan Thamayenthiri Yuvaraj, A. Bhavadharini, K. Senthilkumar, Jan Grzegorz Ma?ecki, Paranthaman Vijayan, P. Viswanathamurthi

#### 140. 3D in situ RuO<sub>2</sub>/ZnO Nanocomposite for Heterogeneous Photocatalytic Degradation of Etoposide in

##### Biological Fluid: Identification of Podophyllotoxin derivatives by LC-HRMS

Surfaces and Interfaces 83, 108539 (February 2026)

V.M. Adhithya Venu, Daniel T. Thangadurai, D. Nataraj, K. Senthilkumar

#### 139. Cyclometallated Ru(II) Complexes Derived from Dibasic CNO Pincer Ligands as Molecular Catalysts for

##### Electrocatalytic Hydrogen Evolution in Alkaline Medium

Inorganic Chemistry 65(5), 3125 -3140 (February 2026)

R. Krishnapriya; V. Monica; A. Bhavadharini, K. Senthilkumar, P. Vijayan, B. Srinivasa, P. Viswanathamurthi

#### 138. Mechanism and kinetics of chlorothalonil reaction with atmospheric oxidants

Computational and Theoretical Chemistry, Volume 1256 (December 2025)

S V Thoshiba, L Sandhiya, K Senthilkumar

#### 137. Influence of Substituents on the Gas-Phase Ozonolysis of Ethene: A Theoretical Study

ChemPhysChem, 00, e202500536 (October 2025)

A. Bhavadharini, L. Sandhiya, and K. Senthilkumar

#### 136. Atmospheric Fate and Emissions of Hydrofluoroether-356pcf3 in Indian Scenario

ACS Earth and Space Chemistry, 9, 2260-2271 (August 2025)

Sandhiya Lakshmanan, Vikas Kumar Maurya, G Manonmani, K Senthilkumar

#### 135. The role of pore diameter on tuning the hydrogen storage capacity of Yttrium atom decorated covalent organic frameworks: A theoretical study

Energy storage, Volume 7, issue 4, e70177 (May 2025)

V. M. Vasanthakannan, K. Senthilkumar

#### 134. Biopermissible and Hydrophilic G-CNNPs for Noncooperative Binding with Picomolar of Cancer Drug

##### Etoposide and Photodynamic Therapy

ACS Applied Bio materials, 8, 4351-4366 (April 2025)

Anusree S. Gangadharan, Daniel T. Thangadurai, V. M. Vasanthakannan, K. Senthilkumar and D. Nataraj



## 133. OH Radical-Initiated Oxidation of 1-Dimethylamino-2-Nitroethylene: A Theoretical Study

ChemistrySelect, Volume10, Issue7, e202401821 (February 2025)  
S. V. Thoshiba, L Sandhiya, K Senthilkumar

## 132. Copper (I) complexes with heteroaromatic hydrazone ligands: Synthesis, crystal structure and catalytic insights for tetrazole synthesis

Inorganica Chimica ActaVolume 575, 122418 (January 2025)  
S Gayathri, P Viswanathamurthi, JG Malecki, A Bhavadharini, K Senthilkumar

## 131. A combined experimental and theoretical studies on organic single crystal diguanidinium squarate dihydrate for nonlinear optical applications

Journal of the Indian Chemical SocietyVolume 102, Issue 3, 101594 (January 2025)  
E Manjula, Suba Chandrasekar, A Bhavadharini, K Senthilkumar, S Janani, G Vinitha, P Murugakoothan

## 130. Unraveling the Autoxidation Mechanisms of Limonene, $\alpha$ -Pinene, and $\beta$ -Pinene: A Computational Study with Reactivity Prediction Models

The Journal of Physical Chemistry A 10609-10619 (December 2024)  
A Bhavadharini, L Sandhiya, K Senthilkumar

## 129. Surface-designed AuNPs-based fluorescent Probe for ultra-sensitive detection of oral poultry antibacterial drug furaltadone via Intermolecular hydrogen bonding

RSC Advances, 14 (2024) 28224 (September 2024)  
A. Sowndarya, T. Daniel Thangadurai, N. Manjubaashini, M. Pavithrakumar, K. Senthilkumar, D. Nataraj, K Kadirvelu, K. Naveen kalagatur

## 128. Quasi-Spherical and Upconversion g-CNNPs for Ultrasensitive Detection of Fipronil in Soil Samples and Bioimaging in Zebrafish

ACS Appl. Nano Mater. 18, 21388–21400 (September 2024)  
Anusree S Gangadharan, Daniel T Thangadurai, Kittusamy Senthilkumar, Valarmani M Vasanthakannan, Nandhakumar Manjubaashini, Devaraj Nataraj, Naveen K Kalagatur

## 127. Hydrogen storage property of the Sc decorated aza-triphenylene based covalent organic framework

Journal of Power SourcesVolume 604,234505 (June 2024)  
V. M. Vasanthakannan, K Senthilkumar

## 126. Triselenasumanene-based organic molecules as donor and hole transporting materials for next-generation solar cells

Journal of Physics and Chemistry of Solids, 190, 111961 (March 2024)  
M. Pavithrakumar and K. Senthilkumar

## 125. First principle studies on triphenylene-hexathiol-based metal-organic framework for hydrogen storage application

Journal of Energy Storage, 78, 110077 (February 2024)  
V.M. Vasanthakannan, M. Pavithrakumar, K. Senthilkumar

## 124. Theoretical investigations of the substituent effect on the opto-electronic properties of the linearly fused naphthadithiophene-based molecules

The Journal of Computational Chemistry 45, 915 (January 2024)  
Jothi Balakrishnan, Pavithrakumar Muthukumar, David Stephen Arputharaj, Pitchumani Violet Mary Christopher, Selvaraju Karuppannan, Senthilkumar Kittusamy

## 123. The association of air quality and complex atmospheric oxidation chemistry in the dispersion and deposition of SARS-CoV-2-laden aerosols

Environmental Science: Advances, 2(11), 1540-1553. (September 2023)  
Sandhiya Lakshmanan, Ranjana Aggarwal, Kittusamy Senthilkumar, Anupama Upadhyay

## 122. Reaction of Criegee Intermediates with SO<sub>2</sub>? A Possible Route for Sulfurous Acid Formation in the Atmosphere

ACS Earth and Space Chemistry, 7(10),1890-1904. (September 2023)  
Manonmani, G., Sandhiya, L. and Senthilkumar, K.



## 121. New insights into pertinent Fe-complexes for the synthesis of iron via the instant polyol process

Physical Chemistry Chemical Physics, 25(33), 21970-21980 (August 2023)  
Sivaranjani Kottaipalayam Somasundaram, Ana Guilherme Buzanich, Franziska Emmerling, Sangameswaran Krishnan, Kittusamy Senthilkumar, Raphael Justin Joseyphus

## 120. Tailoring the mechanistic pathways and kinetics of OH-addition reaction of sulfoxaflo and its ecotoxicity assessment

Environmental Science and Pollution Research, 30(17), 50209-50224 (February 2023)  
G Manonmani, L Sandhiya, K Senthilkumar

## 119. A Computational Perspective on the Chemical Reaction of HFO-1234zc with the OH Radical in the Gas Phase and in the Presence of Mineral Dust

J. Phys. Chem. A 126, 51, 9564–9576 (December 2022)  
G. Manonmani, L. Sandhiya, and K. Senthilkumar

## 118. Nitrogen- and Boron-Doped Polycyclic Aromatic Hydrocarbons as Hole Transporting Materials for Perovskite Solar Cells

Journal of Electronic Materials, 52, 1461–1473 (December 2022)  
M. Pavithrakumar and K. Senthilkumar

## 117. Opto-Electronic Properties of Quasi-Planar Boron clusters–A DFT Investigation

Chemical Physics Letters, 139914 (August 2022)  
S Krishnan, K Senthilkumar

## 116. Tetrathiafulvalene Derivatives as Hole-Transporting Materials in Perovskite Solar Cell

The Journal of Physical Chemistry A, 126, 31, 5079–5088 (August 2022)  
S Krishnan, K Senthilkumar

## 115. Coordination Behavior of Acylthiourea Ligands in Their Ru (II)–Benzene Complexes? Structures and Anticancer Activity

Organometallics, 41, 13, 1621-1630 (June 2022)  
Srividya Swaminathan, Jebiti Haribabu, Mohamed Kasim Mohamed Subarkhan, Gunasekaran Manonmani, Kittusamy Senthilkumar, Nithya Balakrishnan, Nattamai Bhuvanesh, Cesar Echeverria, Ramasamy Karvembu

## 114. Modified Fullerenes as an Acceptor in Bulk Heterojunction Organic Solar Cell – A Theoretical study

Physical Chemistry Chemical Physics, 2021, 23, 27468 - 27476 (November 2021)  
S. Krishnan and K. Senthilkumar

## 113. Mechanism, kinetics and Ecotoxicity Assesment of OH- initiated oxidation reactions of sulfoxaflo

Journal of Physical Chemistry A 125, 46, 10052-10064 (November 2021)  
G. Manonmani, L. Sandhiya and K. Senthilkumar

## 112. A Comparative investigation on the scavenging of 2, 2-diphenyl-1-picrylhydrazyl radical by the natural antioxidants (+) catechin and (-) epicatechin

Journal of Molecular Structure, 1242, 130805 (October 2021)  
S Anitha, S Krishnan, K Senthilkumar, V Sasirekha

## 111. Room temperature weakly ferromagnetic energy band opened graphene quantum dot coupled solid sheets - A possible carbon based dilute magnetic semiconductor

Applied Surface Science 548,149195 (May 2021)  
G. Bharathi, D. Nataraj, O. Y. Khyzhun, D.T. Thangadurai, K. Senthilkumar, M. Sowmiya, R. Kathiresan, P. Kolandaivel, M. Gupta, D. Phase, N. Patra, S. N. Jha, D. Bhattacharyya

## 110. Investigation on Surface interaction between Graphene Nanobuds and Cerium(III) via Fluorescence excimer, Theoretical, Real water sample, and Bioimaging studies

Materials Chemistry and Physics 264, 124453 (May 2021)  
V.R.Pavithra, T. D. Thangadurai, G. Manonmani, K. Senthilkumar, D. Nataraj, J.Jiya, K. Nandakumar and S. Thomas



## 109. Charge Transport and Optical Absorption Properties of Dibenzocoronene Tetracarboxdiimide Based

### Liquid Crystalline Molecules A Theoretical Study

Journal of Physical Chemistry A 125, 3852-3862 (May 2021)

M. Pavithrakumar, S. Krishnan and K. Senthilkumar

## 108. Influence of shape and configuration of a sensitizer molecule on the efficiency of DSSC -A Theoretical

### insight

RSC Advances 11, 5556-5567 (January 2021)

. Krishnan and K. Senthilkumar

## 107. Aggregation induced emission behavior in oleylamine acetone system and its application to get improved

### photocurrent from In2S3 quantum dots

Nature Scientific Reports 10, 19712 (November 2020)

S. Ramya, D. Nataraj, S. Krishnan, S. Premkumar, T. Thrupthia, A. Sangeetha, K. Senthilkumar and T. D. Thangadurai

## 106. Unimolecular Decomposition of Acetyl Peroxy Radical: A Potential Source for Tropospheric Ketene

Physical Chemistry and Chemical Physics 22, 26819-26827 (November 2020)

L. Sandhiya and K. Senthilkumar

## 105. Insight into the Photophysics of Dual Strong Emission (Blue & Green) Producing Graphene Quantum Dot

### Clusters and their Application Towards Selective and Sensitive Detection of Trace Level Fe3+ and Cr6+ Ions

RSC Advances 10, 26613-26630 (July 2020)

G. Bharathi, D. Nataraj, S. Premkumar, P. Saravanan, D. T. Thangadurai, O. Khyzhun, K. Senthilkumar, P. Kathiresan,, P. Kolandaivel, M. Gupta and D. Phase

## 104. Adsorption of phenanthroline and its derivatives on Au (111) surface – Influence of substitution on

### structure and electronic properties

Computational Materials Science 182, 109778 (May 2020)

M.Vinodha, S.Krishnan, S.Bagyalakshmi and K.Senthilkumar

## 103. Theoretical investigation on the structure and antioxidant activity of (+) catechin and (?) epicatechin – a

### comparative study

Molecular Physics, 118, e1745917 (March 2020)

S. Anitha , S. Krishnan , K. Senthilkumar and V. Sasirekha

## 102. Hydrolysis of HNSO2: A Potential Route for Atmospheric Production of H2SO4 and NH3

International Journal of Quantum Chemistry 120, e26182 (February 2020)

G. Manonmani, L. Sandhiya and K. Senthilkumar

## 101. First Principle Studies on the Atmospheric Oxidation of HFC-C1436 Initiated by OH radical

New Journal of Chemistry 44, 2070-2082 (January 2020)

R. Bhuvaneshwari and K. Senthilkumar

## 100. Mechanism and kinetics of Diuron Oxidation by Hydroxyl Radical Addition Reaction

Environmental Science and Pollution Research 27 (2020) 12080-12095 (January 2020)

G. Manonmani, L. Sandhiya and K. Senthilkumar

## 99. Effect of Site Energy Fluctuation on Charge Transport in Disordered Organic Molecules

Journal Chemical Physics 151, 224301 (December 2019)

K. Navamani, Swapan K. Pati, and K. Senthilkumar

## 98. A comprehensive quantum chemical study on the mechanism and kinetics of atmospheric reactions of

### 3-Chloro-2-methyl-1-propene with OH radical

Theoretical Chemistry Accounts 139, 2 (November 2019)

R. Bhuvaneshwari and K. Senthilkumar

## 97. Atmospheric Oxidation Mechanism and Kinetics of 2-Bromo-4, 6-dinitroaniline by OH radical – A

### Theoretical Study

Physical Chemistry and Chemical Physics 21, 21109-21127 (September 2019)

M. Gnanaprakasam, G.Saranya, S. Bandaru, N. JOURNAL English and K. Senthilkumar



## 96. Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical – Hydrogen and Chlorine Atom

### Abstraction Reactions

Journal of Physical Chemistry A 123, 8954-8967 (September 2019)

G. Manonmani, L. Sandhiya and K. Senthilkumar

## 95. Graphene Nanobuds: A New Second-Generation Phosgene Sensor with Ultralow Detection Limit in

### Aqueous Solution

ACS Applied Materials & Interfaces 11 19339-19349 (May 2019)

P.V. Ravi, D. T. Thangadurai, D. Nataraj, K. Senthilkumar, G. Manonmani, N. Kalarikkal, S. Thomas, P. Govindh

## 94. Theoretical Study on the Gas Phase Reaction of Methyl Chavicol with Hydroxyl Radical

Computational and Theoretical Chemistry 1151, 78-90 (March 2019)

R. Bhuvaneswari and K. Senthilkumar

## 93. Adsorption of Tetracyanoquinodimethane and Tetrathiafulvalene on Aluminium (100) surface - A First

### Principle Study of Structural and Electronic Properties

Journal of Molecular Simulation 45, 492-500 (December 2018)

M. Vinodha and K. Senthilkumar

## 92. Mechanism and Kinetics of the Oxidation of Dimethyl Carbonate by Hydroxyl Radical in the Atmosphere

Environmental Science and Pollution Research 26, 3357-3367 (December 2018)

M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

## 91. Theoretical Investigation on the Mechanism and Kinetics of Atmospheric Reaction of

### Methyldichloroacetate with Hydroxyl Radical

Journal of Physical Chemistry A 122. 9316-9325 (October 2018)

M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

## 90. Theoretical probe on modified organic dyes for high-performance Dye-Sensitized Solar Cell

Current Applied Physics 18, 1071-1079 (September 2018)

S. Krishnan and K. Senthilkumar

## 89. Mechanism and kinetics of the reaction of methyl acetate with Cl atom – A theoretical study

Computational and Theoretical Chemistry 1131, 40–50 (May 2018)

M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

## 88. Atmospheric Oxidation Mechanism and Kinetics of Hydrofluoroethers CH<sub>3</sub>OCF<sub>3</sub>, CH<sub>3</sub>OCHF<sub>2</sub> and

### CHF<sub>2</sub>OCH<sub>2</sub>CF<sub>3</sub> by OH Radical: A Theoretical Study

Journal of Physical Chemistry A 122. 4972-4982 (May 2018)

S. Ponnusamy, L. Sandhiya and K. Senthilkumar

## 87. Mechanism and Kinetics of the Degradation of Terbacil initiated by OH radical - A Theoretical Study

Chemical Physics 501, 110-120 (February 2018)

S. Ponnusamy, L. Sandhiya and K. Senthilkumar

## 86. Theoretical and experimental evaluation of a new organic proton transfer crystal aminoguanidinium p-

### nitrobenzoate monohydrate for optical limiting applications

Journal of Physics and Chemistry of Solids 111, 82-94 (December 2017)

T. Shanmugavadivu, K. Senthilkumar, P. Muthuraja, S. Balachandar and M. Sethu Raman

## 85. Counter anion effect on structural, opto-electronic and charge transport properties of fused $\pi$ -conjugated

### imidazolium compound

Molecular Physics 116, 1145-1152 (December 2017)

M. Vinodha and K. Senthilkumar

## 84. Exploring the Mechanisms for the Radical Induced Damage of 6-Thioguanine

International Journal of Quantum Chemistry 118. e25544 (November 2017)

L. Sandhiya and K. Senthilkumar



**83. A theoretical investigation on the mechanism and kinetics of the gas-phase reaction of naphthalene with OH radical**

Theoretical Chemistry Accounts 136, 131 (October 2017)  
M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar

**82. Conversion of toluene into benzyl radical on Anatase TiO<sub>2</sub> (001) surface**

Computational and Theoretical Chemistry 1115, 13-21 (September 2017)  
M..Sowmiya and K. Senthilkumar

**81. Opto-electronic and interfacial charge transfer properties of azobenzene dyes on Anatase TiO<sub>2</sub> (001) surface -The effect of anchoring group**

Journal of Photochemistry and Photobiology A: Chemistry 346, 372-381 (September 2017)  
M..Sowmiya and K. Senthilkumar

**80. Graphene quantum dot solid sheets: strong blue-light-emitting & photocurrent-producing band-gap-opened nanostructures**

Nature - Scientific Reports 7, 10850 (September 2017)  
G. Bharathi, D. Nataraj, P. Sellan, M. Sowmiya, K. Senthilkumar, T. D. Thangadurai, O.Khyzhun, M. Gupta, D. Phase, N. Patra, S. Jha, and D. Bhattacharyya

**79. Ab initio QM/MM modelling of the rate-limiting proton transfer step in the deamination of tryptamine by aromatic amine dehydrogenase**

Journal of Physical Chemistry B 121, 9785-9798 (September 2017)  
K. E. Ranaghan, W. G. Morris, L. Masgrau, K. Senthilkumar, L. O. Johannissen, N. S. Scrutton, J.N. Harvey, F. R. Manby and A. J. Mulholland

**78. Atmospheric oxidation mechanism and kinetics of 1, 3, 5-Trimethylbenzene initiated by OH radical - A theoretical study**

New Journal of Chemistry 41, 10259-10271 (August 2017)  
S. Ponnusamy, L. Sandhiya and K. Senthilkumar

**77. Theoretical investigations on the mechanism and kinetics of OH radical initiated reactions of mono chloroacetic acid**

Journal of Physical Chemistry A, 121, 6028-6035 (July 2017)  
R. Bhuvaneshwari, L. Sandhiya and K. Senthilkumar

**76. Mechanism and kinetics of the reaction of nitrosamines with OH radical - A theoretical study**

International Journal of Chemical kinetics 49, 339-353 (March 2017)  
S. Ponnusamy, L. Sandhiya and K. Senthilkumar

**75. Synthesis, structural characterisation, DNA/ protein binding and in vitro cytotoxicity of three structurally different organorutheniummetallates from single pot**

Journal of Organometallic Chemistry 825-826, 83-99 (October 2016)  
R. Prabhakaran, P. Kalaivani, K. Senthilkumar and K. Natarajan

**74. Atmospheric oxidation mechanism of OH-initiated reactions of diethyl ether – The fate of 1-ethoxy ethoxy radical**

RSC Advances 6, 81354-81363 (August 2016)  
L. Sandhiya, S. Ponnusamy and K. Senthilkumar

**73. Dissociation of N<sub>2</sub>O on Anatase TiO<sub>2</sub> (001) surface - The effect of oxygen vacancy and presence of Ag cluster**

Applied Surface Science 389, 1220-1232, (August 2016)  
M.Sowmiya and K. Senthilkumar

**72. Structural diversity in aroylthiourea copper complexes – formation and biological evaluation of [Cu(I)(μ-S)SCI]<sub>2</sub>, cis-Cu(II)S<sub>2</sub>O<sub>2</sub>, trans-Cu(II)S<sub>2</sub>O<sub>2</sub> and Cu(I)S<sub>3</sub> cores**

New journal of chemistry 40, 5401-5413 (April 2016)  
N. Selvakumaran, L. Sandhiya, N.S.P. Bhuvanesh, K. Senthilkumar and R. Karvembu



## 71. N-Heterocycles as corrosion inhibitors for mild steel in acid medium

Journal of Molecular Liquids 216, 42-52 (January 2016)

J. Saranya, M. Sowmiya, P. Sounthari, K. Parameswari, S. Chitra and K. Senthilkumar

## 70. Adsorption of proline, hydroxyproline and glycine on anatase (001) surface - A first principle study

Theoretical Chemistry Accounts 135, 12 (December 2015)

M.Sowmiya and K. Senthilkumar

## 69. Adsorption of RGD Tripeptide on Anatase (001) Surface - A First Principle Study

Computational Materials Science 104, 124-129 (June 2015)

M.Sowmiya and K. Senthilkumar

## 68. Forth-back oscillated charge carrier motion in dynamically disordered hexathienocoronene molecules: A theoretical study

Physical Chemistry and Chemical Physics 17, 17729-17738 (June 2015)

K. Navamani and K. Senthilkumar

## 67. Effect of dynamic disorder on charge carrier dynamics in Ph4DP and Ph4DTP molecules

RSC Advances 5, 38722-38732 (April 2015)

K. Navamani and K. Senthilkumar

## 66. Ultrasonic, DFT and FT-IR studies on hydrogen bonding interactions in aqueous solutions of diethylene glycol

Journal of Molecular Liquids 202, 115-124, (December 2014)

M. Sethu Raman, M. Kesavan, K. Senthilkumar and V. Ponnuswamy

## 65. Effect of structural fluctuations on charge carrier dynamics in triazene based octupolar molecules

Journal of Physical Chemistry C 118, 27754-27762 (November 2014)

K. Navamani and K. Senthilkumar

## 64. Theoretical studies on the quinoidalthiophene based dyes for dye sensitized solar cell and NLO applications

Physical Chemistry and Chemical Physics 16, 21496-21505 (August 2014)

R.Nithya and K. Senthilkumar

## 63. Mechanism and kinetics of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical

Structural Chemistry 25, 1773-1783 (June 2014)

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## 62. A theoretical probe on the non-covalent interactions of sulfadoxine drug with pi-acceptors

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RSC Advances 4, 25969-25982 (May 2014)

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**54. Structure and spectral properties of L-histidiniumdipicratedihydrate**

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**51. Effect of structural fluctuations on charge carrier mobility in thiophene, thiazole and thiazolothiazole based oligomers**

Physical Chemistry and Chemical Physics 15, 17947-17961 (July 2013)  
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**50. Mechanism and kinetics of the atmospheric oxidative degradation of dimethylphenol isomers initiated by OH radical**

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**49. Opto-electronic properties of low band-gap fused ring thieno[3,4-b]pyrazine analogues - A theoretical study**

Molecular Physics 111, 3036-3046 (February 2013)  
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**48. Theoretical and experimental studies on the structure and spectroscopic properties of Ni(II) complexes of the type [Ni(L) (PPh<sub>3</sub>)] [H<sub>2</sub>L = 5-methyl-N-(2-mercaptophenyl)salicylideneimine and 5-chloro-N-(2-mercaptophenyl)salicylideneimine**

Journal of Molecular Structure 1037, 367-375 (January 2013)  
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**47. Structural properties and the effect of platinum drugs with DNA base pairs**

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**46. A theoretical study of structural and electronic properties of Pentacene/Al(100) interface**

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**45. Reaction Mechanism and kinetics of the atmospheric oxidation of 1,4-thioxane by NO<sub>3</sub> – A theoretical study**

Canadian Journal of Chemistry 90, 384-394 (March 2012)  
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**44. Copper ion mediated selective cleavage of C-S bond in ferrocenylthiosemicarbazone forming mixed geometrical-S)2Cu(PPh3)2] having Cu2S2 core: Towards a new avenue in copper-sulfur chemistry**

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**43. Understanding the absorption and emission spectra of borondipyrromethene dye and its substituted analogs**

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**41. Mechanism and Kinetics of the reaction of 1,4-thioxane with O3 in the atmosphere-A theoretical Study**

Chemical Physics Letters 525-526, 153-159 (January 2012)

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**40. Theoretical investigation of interaction between psoralen and altretamine with stacked DNA base pairs**

Materials Science and Engineering C, 32, 423-431 (December 2011)

P. Deepa, P. Kolandaivel, K. Senthilkumar

**39. Optical Absorption and Emission Properties of Fluoranthene, Benzo[k]fluoranthene, and their Derivatives.**

**A DFT Study**

Journal of Physical Chemistry A 115, 14647-14656 (November 2011)

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**38. Hydrogen bonding studies of Amino acid side chains with DNA base pairs**

Molecular Physics 109, 1995-2008 (August 2011)

P. Deepa, P. Kolandaivel and K. Senthilkumar

**37. Structural Properties and the effect of interaction of alkali (Li+, Na+, K+) and alkaline earth (Be2+, Mg2+, Ca2+) metal cations with G and SG- tetrads**

Computational Theoretical Chemistry 974, 57-65 (July 2011)

P. Deepa, P. Kolandaivel and K. Senthilkumar

**36. Copper(I) hydrazone complexes: Synthesis, structure, DNA binding, radical scavenging and computational studies**

Inorganic Chemical Communications 14, 1318-1322 (May 2011)

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**35. Structural and Spectral Properties of 4-Bromo-1-naphthyl Chalcones: A Quantum Chemical Study**

Journal of Physical Chemistry A 115, 6594-6602 (May 2011)

R. Nithya, N. Santhanamoorthi, P. Kolandaivel, and K. Senthilkumar

**34. Charge Transport and Optical Properties of Discotic Liquid Crystalline Molecules THDDP and Substituted THDP**

International Journal of Quantum Chemistry 112,713-723 (April 2011)

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**33. Hydrogen bond interactions in hydrated acetylsalicylic acid**

Computational Theoretical Chemistry 966, 167-179 (March 2011)

M. Karthika, K. Senthilkumar and R. Kanakaraju

**32. First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes – Ab initio and DFT study**

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International Journal of Quantum Chemistry 111,3482-3496 (October 2010)  
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**28. Tautomerization and solvent effects on the absorption and emission properties of the Schiff base N,N'-bis(salicylidene)- p-phenylenediamine - A TDDFT study**

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International Journal of Quantum Chemistry 110, 1660-1674 (October 2009)  
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**23. Calculation of ionization potential and chemical hardness: A comparative study of different methods**

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**22. Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds**

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V. Sathyabama, M. Karthika, K. Senthilkumar, K. Anandan and R. Kanakaraju

**18. Charge transfer in polypeptides: Effect of secondary structures on charge transfer integral and site-energies**

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## 17. Two dimensional charge delocalization in X-shaped phenylenevinylene oligomers

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### diaminepyridine complexes – A density functional theory study

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Journal of Molecular Structure (Theochem) 589-590,95-102 (August 2002)

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## 7. Hartree-Fock and density functional theory studies on ionization and fragmentation of halomethane molecules by positron impact

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## 6. Quantum chemical studies on tautomerism of barbituric acid in gas phase and in solution

Journal of Computer Aided Molecular Design 16, 263-272 (April 2002)

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## 5. Post Hartree-Fock and density functional theory studies on structure and conformational stability of nitrosoethylene and substituted compounds of nitrosoethylene

Computers and Chemistry 26, 207-221 (January 2002)

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#### 4. Molecular structure, conformational stability and cis effect of 1,4-dichlorobutadiene - A quantum chemical study

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#### 3. Ab initio and DFT studies on structure and stability of aliphatic aldoxime molecules

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#### 2. Studies of chemical hardness and Fukui function using the exact solution of the density functional theory

International Journal of Quantum Chemistry, 81, 4-10 (November 2000)  
K. Senthilkumar, M. Ramaswamy and P. Kolandaivel

#### 1. Study of chemical bonding in H<sub>2</sub> and HF molecule- Wave function and density functional theory (DFT) parameters approach

International Journal of Quantum Chemistry 76, 662-669 (February 2000)  
P. Kolandaivel , N. Suba and K. Senthilkumar

#### Books/Chapters - 3

##### 3. Performance of DFT on open-shell species - case studies from atmospheric chemical reactions

Theoretical and Computational Chemistry - Density Functional Theory - Current Trends and Applications, Elsevier, Volume 25, Pages 333 - 347 ISBN: 978-0-443-18977-7 (October 2025)  
L. Sandhiya and K. Senthilkumar

##### 2. Theoretical Studies on Adsorption of Organic Molecules on Metal Surface

Computational Chemistry Methodology in Structural Biology and Materials Sciences, Apple Academic Press, 209-241, ISBN: 9781771885683 (March 2017)  
G. Saranya and K. Senthilkumar

##### 1. Theoretical Studies on mechanism and kinetics of atmospheric chemical reactions

Reaction Rate Constant Computations: Theories and Applications, Royal Society of Chemistry, 462-493, ISBN: 978-1-84973-650-3 (October 2013)  
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#### Conferences - 11

##### 11. Computational Methods for Molecules and Materials

Resource Person - National Workshop on Emerging Applications of Computational Materials Science and Structural Analysis , Organized by Dept. of Physics , PSG College of Arts & Science, Coimbatore (September 2025)  
K. Senthilkumar

##### 10. Computational methods for molecules and materials

Resource Person - Workshop on from theory to simulation: A hands-on course on G16 and VASP for materials research, organized by Center for Computational Physics, Dept. of Physics, Karpagam Academy of Higher Education, Coimbatore (May 2025)  
K. Senthilkumar

##### 9. Computational methods for molecules and materials

Resource Person - DST-ANRF sponsored three days national seminar on Emerging Predictive Modelling in Material Science, organized by Hindusthan Institute of Technology, Coimbatore (April 2025)  
K. Senthilkumar

##### 8. National Science day address

Hindusthan Institute of Technology, Coimbatore (February 2025)  
K. Senthilkumar

##### 7. Theoretical studies on the hydrogen adsorption properties of transition metal decorated covalent organic framework.

10th Virtual International Conference on Science, Technology and Management in Energy - eNergetics 2024. (November 2024)  
V. M. Vasanthakannan, K. Senthilkumar



## 6. Finding suitable materials for next-generation solar cells

National Level Workshop cum Faculty Development Programme on Computational Methods for Solving Chemical Problems, National Institute of Technology Tiruchirappalli, Tamil Nadu (February 2024)

K. Senthilkumar

## 5. Reaction of Criegee intermediates with SO<sub>2</sub> - A possible route for sulfurous acid formation in the atmosphere

Theoretical Chemistry symposium (TCS-2023), Indian Institute of Technology - Madras, Chennai (December 2023)

K. Senthilkumar

## 4. Improving the performance of perovskite solar cells by surface passivation of amino acids: A theoretical study

Theoretical Chemistry symposium (TCS-2023), Indian Institute of Technology - Madras, Chennai (December 2023)

M. Pavithrakumar and K. Senthilkumar

## 3. Hydrogen storage property of the Sc decorated aza-triphenylene based covalent organic framework

Theoretical Chemistry symposium (TCS-2023), Indian Institute of Technology - Madras, Chennai (December 2023)

V. M. Vasanthakannan and K. Senthilkumar

## 2. Unravelling the autoxidation mechanisms of alpha-pinene and limonene: A computational study with reactivity predictions

Theoretical Chemistry symposium (TCS-2023), Indian Institute of Technology - Madras, Chennai (December 2023)

A. Bhavadharini and K. Senthilkumar

## 1. Mechanisms of Hydroxyl Radical Initiated Oxidation of 1-Dimethylamino-2-Nitroethylene: A Computational study

Theoretical Chemistry symposium (TCS-2023), Indian Institute of Technology - Madras, Chennai (December 2023)

S. V. Thoshiba and K. Senthilkumar

## National Journals - 1

### 1. Reaction mechanism and kinetics of the atmospheric reactions of 2,3-dimethylphenol with OH radical

Journal of International Academy of Physical Sciences, 15, 359, (2011) (October 2011)

L. Sandhiya, P. Kolandaivel and K. Senthilkumar

## Patents

### Granted - 1

1. Method to produce graphene quantum dot sheet and its applications 05-2022 397923 Dr. D. Nataraj, Dr. G. Bharathi, Dr. K. Senthilkumar

## Projects

### Completed - 5

1. Probing the mechanism, thermochemistry and kinetics of the degradation of organic air pollutants in the atmosphere TANSCHERs. 21,33,000 (April 2021 - October 2024)
2. Driving perovskite photovoltaics towards next generation solar cells through computational material engineering DST – SERB Rs. 22,69,764 (December 2020 - June 2024)
3. Effect of structural fluctuations and environment on charge transport in  $\pi$ -stacked and conjugated organic molecules DST Rs. 17,87,200 (September 2008 - August 2011)
4. Theoretical studies on charge transport properties in organic field effect transistor UGC-MRP Rs. 7,40,100 (October 2010 - September 2012)
5. Quantum mechanical and molecular mechanical studies on the reactions of pollutants in atmosphere and in water CARS-DRDO Rs. 13,43,800 (July 2012 - June 2015)